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1970 J. Phys. A: Gen. Phys. 3 346

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## An expansion of the master equation with applications to coupled atom-radiation systems

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*MS. received 19th March 1970*

**Abstract.** A straightforward extension of time-dependent quantum-mechanical perturbation theory is made to obtain the equivalent formulae for a statistical mixture of states. The 'master equation' resulting from this procedure is, in its lowest order, the analogue in quantum statistics of the 'Golden Rule' for transition rates and reduces exactly to this form in the limit of pure initial states. We give results to fourth order and illustrate their use by applying them to the problem of the resonant interaction of an electromagnetic field and a two-level atom.

### 1. Introduction

The von Neumann equation of motion for the density matrix might be called the very basis of quantum statistical mechanics. Starting with Pauli in 1928 attempts have been made to process this equation to obtain an equation connecting diagonal elements only and having the gain-loss structure typical of the Boltzmann equation. Such an equation is called a master equation, and derivations have been presented, for example, by Van Hove (1955), Prigogine (1962), Swenson (1962) Zwanzig (1964) and Pike (1965). The mathematical techniques used in these papers are sometimes complex and, although progress has been made (see for example Argyres and Kelley 1964 and Haake 1969), it is not always easy to see how to apply the master equations so derived to real physical systems.

In this paper we present a derivation of an irreversible master equation by a generalization of the methods of ordinary perturbation theory to deal with quantum statistical mechanics. The derivation proceeds in two stages. In the first stage we present the terms to fourth order of the exact time-reversible perturbation expansion for the density matrix. This result is essentially that derived by Pike (1965) using a Fourier-Hilbert transform technique but the derivation here we believe is simpler to follow. In the second stage the essential additional step we make is to introduce a small density-of-states spread onto the levels of the unperturbed system in the equation of motion for the density matrix. Although novel in this context this is entirely equivalent to the procedure described in any text book for obtaining the 'Golden Rule' formula for transition rates for pure states. By integrating in the usual way over these small spreads of states (which do not represent practically observable states of the system) we introduce irreversible behaviour and we are able to derive an equation for the density matrix, which we regard in its lowest order as no more than the 'Golden Rule' for mixed states and in its higher orders as the exact generalization of the higher-order terms of time-dependent perturbation theory for quantum statistical mechanics. This equation is valid over the same time scale as ordinary time-dependent perturbation theory (Dirac 1958—p. 181). From this equation we are able to derive a master equation in terms of course-grained time derivatives of the density matrix.

The density-matrix method has proved to be one of the most fruitful methods of calculating the statistical properties of laser light (see, for example, Fleck 1966, Scully and Lamb 1966, Lax and Louisell 1967 and Wiedlich *et al.* 1967). A knowledge

of the diagonal elements of the density matrix for all time enables one to calculate the dynamic and steady-state values of the intensity of laser light, as well as the statistical distribution of the number of photons in the cavity mode (see Pike 1970 as well as the papers listed above). In the final section of this paper, for illustration, we apply our master equation to the problem of an atom interacting with a cavity mode of electromagnetic radiation in the presence of dissipative reservoir interactions and pumping mechanisms. We are able to derive the equation for the photon number distribution (i.e. the probability that there are  $n$  photons in the field) directly and we compare it with the laser equation of Scully and Lamb.

In § 2 we present the perturbation-theory derivation of the time-reversible equation for the diagonal elements of the density matrix. In § 3 we perform the sum over intermediate states to obtain the time-irreversible equation and we show that, after an appropriately long time, any initial off-diagonal elements of the density matrix make a constant (in time) contribution to the diagonal elements. Provided that this time is not so large that the perturbative method ceases to be valid, or that the master function changes appreciably in this time, we are able to show that the off-diagonal elements make a negligible contribution to the equations of motion for the diagonal elements. In this way we are able to derive a master equation in terms of coarse-grained time derivatives. The functions which satisfy this equation give the averaged time evolution of the density matrix (the meaning of "averaged" in this context is made apparent in § 3). In § 4, as stated above, we apply the master equation to the problem of atom-field interactions.

## 2. The time-reversible equation

We consider a system described by the Hamiltonian

$$H = H_0 + gV \tag{2.1}$$

where  $g$ , the coupling constant, is a small parameter. The eigenstates and eigenvalues of  $H_0$  satisfy the equation

$$H_0|r\rangle = E_r|r\rangle. \tag{2.2}$$

We define our master functions  $P_{rs}(t)$  and  $p_{rs}(t)$  as follows (Pike 1965)

$$P_{rs}(t) = \text{Tr}\{\rho(0) |r(t)\rangle \langle s(t)|\} \tag{2.3}$$

$$P_{rs}(t) = \exp(iE_{rs}t)p_{rs}(t), \quad E_{rs} = E_r - E_s \tag{2.4}$$

where  $\rho(0)$  is the density operator at  $t = 0$ . It obeys the von Neumann equation

$$\frac{d\rho}{dt} = [H, \rho]. \tag{2.5}$$

Equation (2.4) represents a transformation to the interaction picture. The equation of motion for  $p_{rs}(t)$  follows from equations (2.1)–(2.5) and is

$$\frac{dp_{rs}(t)}{dt} = -g \sum_q [p_{qs}(t) V_{qr} \exp(iE_{qr}t) - p_{rq}(t) \exp(iE_{sq}t) V_{sq}]. \tag{2.6}$$

This equation is easily integrated to give

$$p_{rs}(t) - p_{rs}(0) = ig \sum_q \int_0^t dt' [p_{qs}(t') \exp(iE_{qr}t') V_{qr} - p_{rq}(t') \exp(iE_{sq}t') V_{sq}]. \tag{2.7}$$

This is the equation we use as the basis of our perturbation expansion. We adopt a

new notation which makes the equations more concise

$$\Delta p_{rs}(t) = g \sum_q [U_{sq} p_{rq}(t) - U_{qr} p_{qs}(t)] \tag{2.8}$$

where  $U_{sq}$  is the integral operator, operating on functions of  $t$ :

$$U_{sq} f(t) \equiv -i \int_0^t dt' V_{sq} \exp(iE_{sq}t') f(t'). \tag{2.9}$$

We shall encounter expressions of the form  $U_{rq} U_{qs} f(t)$ . These are to be interpreted as

$$(-i)^2 \int_0^t dt' V_{rq} \exp(iE_{rq}t') \int_0^{t'} dt'' V_{qs} \exp(iE_{qs}t'') f(t'').$$

We make the assumption that our master functions can be expanded in series of the form

$$p_{rs}(t) = p_{rr}^{(0)}(t) \delta_{rs} + \sum_{n=1}^{\infty} g^n p_{rs}^{(n)}(t) \quad t \geq 0. \tag{2.10}$$

We have assumed that in the limit  $g \rightarrow 0$  the master functions become diagonal. This would be the case, for instance, if the density matrix were diagonal in the infinite past.

By substituting from (2.10) into (2.8) we obtain the following set of equations:

$$p_{rr}^{(0)}(t) = p_{rr}^{(0)}(0) \tag{2.11}$$

$$p_{rs}^{(1)}(t) - p_{rs}^{(1)}(0) = U_{sr} [p_{rr}^{(0)}(t) - p_{ss}^{(0)}(t)] \tag{2.12}$$

and, for  $n \geq 2$ ,

$$p_{rs}^{(n)}(t) - p_{rs}^{(n)}(0) = \sum_q [U_{sq} p_{rq}^{(n-1)}(t) - U_{qr} p_{qs}^{(n-1)}(t)]. \tag{2.13}$$

One obtains  $p_{rs}^{(1)}(t)$  in terms of master functions evaluated at  $t = 0$  by substituting from (2.11) into (2.12). This expression for  $p_{rs}^{(1)}(t)$  is substituted into equation (2.13) for  $n = 2$  to obtain  $p_{rs}^{(2)}(t)$ , and so on. By these means one can derive an equation for  $p_{rs}(t)$  to any order in terms of the initial  $p_{rs}(0)$ . The result to fourth order may be written as

$$\Delta p_{rs,4}(t) = N_{rs,4}(t) + Q_{rs,4}(t) \tag{2.14}$$

where the notation  $p_{rs,4}(t)$  means the value of  $p_{rs}(t)$  correct to the fourth order, i.e.

$$p_{rs,4}(t) = \sum_{i=0}^4 g^i p_{rs}^{(i)}(t).$$

The first term of the right-hand side of (2.14) is

$$\begin{aligned} N_{rs,4}(t) = & g[U_{sr} p_{rr,3}(0) + \text{h.c.}] + g^2 \sum_{q_1} [U_{sq_1} U_{q_1r} \{p_{q_1q_1,2}(0) - p_{ss,2}(0)\} + \text{h.c.}] \\ & + g^3 \sum_{q_1} \sum_{q_2} [U_{sq_2} U_{q_2q_1} U_{q_1r} \{p_{rr,1}(0) - p_{q_1q_1,1}(0)\} \\ & \quad - U_{sq_2} U_{q_2q_1} U_{q_1r} \{p_{rr,1}(0) - p_{q_2q_2,1}(0)\} + \text{h.c.}] \\ & + g^4 \sum_{q_1} \sum_{q_2} \sum_{q_3} [U_{sq_1} U_{q_1q_2} U_{q_2q_3} U_{q_3r} \{p_{rr,0}(0) - p_{q_3q_3,0}(0)\} \\ & \quad - U_{sq_1} U_{q_1q_2} U_{q_2q_3} U_{q_3r} \{p_{q_3q_3,0}(0) - p_{q_2q_2,0}(0)\} \\ & \quad - U_{sq_1} U_{q_2r} U_{q_3q_2} U_{q_1q_3} \{p_{q_2q_2,0}(0) - p_{q_3q_3,0}(0)\} \\ & \quad + U_{sq_1} U_{q_2r} U_{q_3q_2} U_{q_1q_3} \{p_{q_2q_2,0}(0) - p_{q_1q_1,0}(0)\} + \text{h.c.}] \tag{2.15} \end{aligned}$$

where +h.c. means add on the term with  $r$  and  $s$  interchanged and the complex conjugate taken. Thus the first-order term above in full is

$$g[U_{sr}p_{rr,3}(0) + U_{rs}^*p_{ss,3}(0)]$$

which is equal to  $gU_{sr}[p_{rr,3}(0) - p_{ss,3}(0)]$  since

$$U_{rs}^* = -U_{sr}.$$

The second term of the right-hand side of (2.14) is

$$\begin{aligned} Q_{rs,4}(t) = & g \left[ \sum_{q_1 \neq r} U_{sq_1} p_{rq_1,3}(0) + \text{h.c.} \right] \\ & + g^2 \sum_{q_2} \left[ \sum_{q_1 \neq r} U_{sq_2} U_{q_2q_1} p_{rq_1,2}(0) - \sum_{q_1 \neq q_2} U_{sq_2} U_{q_1r} p_{q_1q_2,2}(0) + \text{h.c.} \right] \\ & + g^3 \sum_{q_3} \sum_{q_2} \left[ \sum_{q_1 \neq r} U_{sq_3} U_{q_3q_2} U_{q_2q_1} p_{rq_1,1}(0) \right. \\ & \quad - \sum_{q_1 \neq q_2} U_{sq_3} U_{q_3q_2} U_{q_1r} p_{q_1q_2,1}(0) - \sum_{q_1 \neq q_2} U_{sq_3} U_{q_2r} U_{q_3q_1} p_{q_2q_1,1}(0) \\ & \quad \left. + \sum_{q_1 \neq q_3} U_{sq_3} U_{q_3r} U_{q_1q_2} p_{q_1q_3,1}(0) + \text{h.c.} \right]. \end{aligned} \quad (2.16)$$

We have arranged terms so that the  $N_{rs}(t)$  terms contain only diagonal master functions whilst the  $Q_{rs}(t)$  terms contain only off-diagonal master functions. We shall show later that the  $Q_{rs}(t)$  term can be neglected compared with the  $N_{rs}(t)$  term in the long-time limit. (We shall explain the meaning of the long-term limit in § 3.)

Returning to the expression for  $N_{rs}(t)$ , it is clear that its accuracy to order  $g^4$  is unaffected if we replace  $p_{rs,3}(0)$ ,  $p_{rs,2}(0)$  etc. by  $p_{rs}(0)$  given by (2.10) (i.e. the exact initial density matrix). This substitution adds only terms of fifth order in  $g$ .

In the Appendix it is shown that  $N_{rr}(t)$  can be written in the much simplified form

$$\begin{aligned} N_{rr,4}(t) = & -g^2 \sum_{q_1} (U_{rq_1})(U_{q_1r}) [p_{rr}(0) - p_{q_1q_1}(0)] \\ & + g^3 \sum_{q_1} \sum_{q_2} [(U_{q_1r})(U_{rq_2} U_{q_2q_1}) - (U_{rq_1})(U_{q_1q_2} U_{q_2r})] [p_{rr}(0) - p_{q_1q_1}(0)] \\ & + g^4 \sum_{q_1} \sum_{q_2} \sum_{q_3} [U_{rq_3} U_{q_3q_1})(U_{q_2r} U_{q_1q_2}) - (U_{rq_3} U_{q_3q_2} U_{q_2q_1})(U_{q_1r}) \\ & \quad - (U_{rq_1})(U_{q_1q_2} U_{q_2q_3} U_{q_3r})] [p_{rr}(0) - p_{q_1q_1}(0)]. \end{aligned} \quad (2.17)$$

Written in this way, the expression for  $N_{rs}(t)$  closely resembles that obtained in the usual perturbation theory of transition probabilities (see, for example, Dirac 1958—pp. 172–5). Indeed (2.17) reduces to the usual formula for the probability that the system will be in the state  $r$  at time  $t$  if it was certainly in the state  $k$  at time zero. i.e.

$$p_{kk}(0) = 1, \quad p_{qk}(0) = 0, \quad q \neq k.$$

Terms in  $(U_{rq_1})(U_{q_1r})$  and  $(U_{rq_2} U_{q_3q_1})(U_{q_2r} U_{q_1q_2})$  which have an equal number of terms in each bracket we will refer to as ‘direct’ terms by analogy with perturbation theory and terms such as  $(U_{q_1r}) (U_{rq_2} U_{q_2q_1})$  and  $(U_{rq_3} U_{q_3q_2} U_{q_3q_1}) (U_{q_1r})$  we will refer to as ‘interference’ terms.

In the next section we shall introduce the sum over the intermediate states and derive the master equation. We shall show that, in the long-time limit,

$$\Delta p_{rr}(t) \sim N_{rr}(t).$$

After summing over the broadened levels, this will reduce to (again in the long-time limit)

$$\Delta p_{rr}(t) = -t \sum_{q_1} K(t, q_1) [p_{rr}(0) - p_{q_1 q_1}(0)]$$

an equation which exhibits the gain-loss structure referred to in the introduction.

### 3. Broadening of the levels

We wish to generalize our equations to the situation where each eigenvalue  $E_r$ , instead of being sharp and discrete, has associated with it a continuum of eigenvalues labelled by an  $\alpha_r$  (or  $\alpha$  for short). The energies  $\epsilon_\alpha$  of the  $\alpha$ -state are measured from the energy  $E_r$  and are assumed to form a narrow band centred on  $E_r$ . It will be convenient in the later stages to assume that the density of the  $\alpha$ -states has a Lorentzian profile centred on  $E_r$ , i.e.

$$h_r(\alpha) = \frac{\Gamma_r/\pi}{\epsilon_\alpha^2 + \Gamma_r^2} \quad (3.1)$$

where  $h_r(\alpha)$  is the density of the states associated with the  $r$  states and  $\Gamma_r$  is the half-width. We wish to trace over these states to obtain our final equations since they do not represent practically observable states of the system. If we consider as an example an atom interacting with a single mode of radiation, this broadening could be thought of as originating from transitions of the atomic levels being considered to atomic levels of no direct interest, or due to a small spread in frequency of the radiation mode.

Our equations will be changed by this device only to the extent that the label  $r$  must be replaced by the  $r\alpha$ ,  $s$  by  $s\beta$ , etc. Since the broadening is small, we make the further assumptions

$$V_{r\alpha, q\gamma} \simeq V_{rq} \quad (3.2)$$

$$p_{r\alpha, s\beta}(0) \simeq p_{rs}(0). \quad (3.3)$$

The time integrals involved in (2.17) can be written out explicitly as

$$U_{rq_1} = (-1) V_{rq_1} \frac{\exp(iE_{rq_1}t) - 1}{E_{rq_1}} \quad (3.4)$$

$$U_{rq_2} U_{q_2 q_1} = (-1)^2 V_{rq_2} V_{q_2 q_1} \left\{ \frac{\exp(iE_{rq_1}t) - 1}{E_{q_2 q_1} E_{rq_1}} + \frac{\exp(iE_{rq_2}t) - 1}{E_{rq_2} E_{q_1 q_2}} \right\} \quad (3.5)$$

$$U_{rq_3} U_{q_3 q_2} U_{q_3 q_1} = (-1)^3 V_{rq_3} V_{q_3 q_2} V_{q_3 q_1} \left\{ \frac{\exp(iE_{rq_1}t) - 1}{E_{rq_1} E_{q_2 q_1} E_{q_3 q_1}} + \frac{\exp(iE_{rq_2}t) - 1}{E_{rq_2} E_{q_3 q_2} E_{q_1 q_2}} \right. \\ \left. + \frac{\exp(iE_{rq_3}t) - 1}{E_{rq_3} E_{q_2 q_3} E_{q_1 q_3}} \right\}. \quad (3.6)$$

For brevity, we shall treat in detail only the second-order contribution to  $N_{rr}(t)$ , and merely quote the results for higher orders.

From (2.17),

$$N_{rr}^{(2)}(t) = -g^2 \sum_{q_1} (U_{rq_1})(U_{q_1 r}) [p_{rr}(0) - p_{q_1 q_1}(0)].$$

We shall now evaluate this quantity explicitly when level broadening is introduced. Using (2.17), (3.4) and approximations (3.2) and (3.3), we have

$$N_{r\alpha, r\alpha}^{(2)}(t) = -g^2 \sum_{q_1} \int_{-\infty}^{\infty} d\epsilon_\beta |V_{rq_1}|^2 \frac{2[1 - \cos(E_{rq_1} + \epsilon_{\alpha\beta})t]}{(E_{rq_1} + \epsilon_{\alpha\beta})^2} h_q(\epsilon_\beta) [p_{rr}(0) - p_{q_1 q_1}(0)]. \quad (3.7)$$

The integral in equation (3.7) is exactly that encountered in the first-order perturbation theory of transition rates, where one is considering a transition from an initial state to a continuum of final states (see, for example, Schiff 1955—p. 199). In the usual treatment, one assumes that only the pole on the real axis contributes, i.e.

$$I \equiv \int_{-\infty}^{\infty} d\epsilon_\beta h_{q_1}(\epsilon_\beta) \frac{2[1 - \cos(E_{rq_1} + \epsilon_{\alpha\beta})t]}{(E_{rq_1} + \epsilon_{\alpha\beta})^2} \simeq 2\pi t h_{q_1}(E_{rq_1} + \epsilon_\alpha). \quad (3.8)$$

However, it can be evaluated exactly for the spectrum (3.1), and the result is

$$I = \text{Re} \left\{ \frac{2[1 - \exp(-\Gamma_{q_1} t) \exp\{-i(E_{rq_1} + \epsilon_\alpha)t\}]}{\{i\Gamma_{q_1} - (E_{rq_1} + \epsilon_\alpha)\}^2} + \frac{2\pi(\Gamma_{q_1}/\pi)t}{(E_{rq_1} + \epsilon_\alpha)^2 + \Gamma_{q_1}^2} \right\}. \quad (3.9)$$

We are now able to explain what we mean by the long-time limit. We mean for values of  $t$  sufficiently small for perturbation theory to be valid, but sufficiently large that  $\Gamma_{q_1} t \gg 1$ . In this case (3.9) reduces to

$$I \sim 2\pi t \frac{(\Gamma_{q_1}/\pi)}{(E_{rq_1} + \epsilon_\alpha)^2 + \Gamma_{q_1}^2} = 2\pi t h_{q_1}(E_{rq_1} + \epsilon_\alpha)$$

as in (3.8).

Substituting for  $I$  from (3.8) into (3.7), we have

$$N_{r\alpha, r\alpha}^{(2)}(t) \simeq -2\pi g^2 t \sum_{q_1} |V_{rq_1}|^2 h_{q_1}(E_{rq_1} + \epsilon_\alpha) [p_{rr}(0) - p_{q_1 q_1}(0)]. \quad (3.10)$$

This equation still contains the unwanted  $\alpha$ 's. The quantity of real physical interest is

$$\int_{-\infty}^{\infty} h_r(\epsilon_\alpha) d\epsilon_\alpha N_{r\alpha, r\alpha}^{(2)}(t) = N_r^{(2)}(t) = -g^2 t \sum_{q_1} |V_{rq_1}|^2 h(rq_1) [p_{rr}(0) - p_{q_1 q_1}(0)] \quad (3.11)$$

using (3.10), where we have defined

$$h(rq_1) = 2\pi \int_{-\infty}^{\infty} h_r(\epsilon_\alpha) h_{q_1}(E_{rq_1} + \epsilon_\alpha) d\epsilon_\alpha. \quad (3.12)$$

For two Lorentzians, this integral is easily evaluated and the result is

$$h(rq_1) = \frac{2\pi(\Gamma_{rq_1}/\pi)}{E_{rq_1}^2 + \Gamma_{rq_1}^2}, \quad \Gamma_{rq_1} \equiv \Gamma_r + \Gamma_{q_1}. \quad (3.13)$$

Defining  $\Delta p_r(t)$  and  $Q_r(t)$  analogously to  $N_r(t)$  in equation (3.11) and calculating to fourth order we find that

$$\Delta p_r(t) = -t \sum_{q_1} K(r, q_1) [p_{rr}(0) - p_{q_1 q_1}(0)] + Q_r(t) \quad (3.14)$$

where

$$\begin{aligned}
 K(r, q_1) &= g^2 |V_{rq_1}|^2 h(r, q_1) \\
 &+ g^3 \sum_{q_2} \{h(r, q_1 q_2) V_{q_1 r} V_{rq_2} V_{q_2 q_1} + h^*(r, q_1 q_2) V_{rq_1} V_{q_1 q_2} V_{q_2 r}\} \\
 &+ g^4 \sum_{q_2 q_3} \{ \bar{h}(r, q_1 q_2 q_3) V_{rq_3} V_{q_3 q_1} V_{q_1 q_2} V_{q_2 r} - V_{rq_3} V_{q_3 q_2} V_{q_2 q_1} V_{q_1 r} h(r, q_1 q_2 q_3) \\
 &\quad - h^*(r, q_1 q_2 q_3) V_{rq_1} V_{q_1 q_2} V_{q_2 q_3} V_{q_3 r} \}. \tag{3.15}
 \end{aligned}$$

We have defined

$$h(r, q_1 q_2) = 2\pi \int_{-\infty}^{\infty} d\epsilon_\alpha h_r(\epsilon_\alpha) h_{q_1}(E_{rq_1} + E_\alpha) \int_c \frac{d\epsilon_\gamma h_{q_2}(\epsilon_\gamma)}{E_{q_2 r} + E_{\gamma\alpha}} \tag{3.16}$$

where  $c$  is a contour which lies along the real axis except for passing beneath the pole at  $\epsilon_{\gamma\alpha} + E_{q_2 r} = 0$ ; similarly,

$$h(r, q_1 q_2 q_3) = 2\pi \int_{-\infty}^{\infty} d\epsilon_\alpha h_r(\epsilon_\alpha) h_{q_1}(E_{rq_1} + \epsilon_\alpha) \int_c \frac{h_{q_3}(E_\delta) d\epsilon_\delta}{E_{q_3 r} + \epsilon_{\delta\alpha}} \int_c \frac{h_{q_2}(\epsilon_\gamma) d\epsilon_\gamma}{E_{q_2 r} + \epsilon_{\gamma\alpha}} \tag{3.17}$$

$$\bar{h}(r, q_1 q_2 q_3) = 2\pi \int_{-\infty}^{\infty} d\epsilon_\alpha h_r(\epsilon_\alpha) h_{q_1}(E_{rq_1} + \epsilon_\alpha) \int_c \frac{h_{q_3}(E_\delta) d\epsilon_\delta}{E_{q_3 r} + \epsilon_{\delta\alpha}} \left\{ \int_c \frac{h_{q_2}(\epsilon_\gamma) d\epsilon_\gamma}{E_{q_2 r} + \epsilon_{\gamma\alpha}} \right\}^* \tag{3.18}$$

Equations (3.16), (3.17) and (3.18), when evaluated for the case of Lorentzian profiles, as was done in (3.13) above, are

$$\begin{aligned}
 h(r, q_1 q_2) &= i \left[ \frac{1}{\Gamma_{r1} \Gamma_{2r}} + \frac{1}{\Gamma_{r1} \Gamma_{21}} + \frac{1}{\Gamma_{2r} \Gamma_{21}} \right] \\
 h(r, q_1 q_2 q_3) &= - \left[ \frac{1}{\Gamma_{r1} \Gamma_{3r} \Gamma_{2r}} + \frac{1}{\Gamma_{r1} \Gamma_{31} \Gamma_{21}} + \frac{1}{\Gamma_{3r} \Gamma_{2r} \Gamma_{31}} + \frac{1}{\Gamma_{2r} \Gamma_{31} \Gamma_{21}} \right]
 \end{aligned}$$

and

$$\begin{aligned}
 \bar{h}(r, q_1 q_2 q_3) &= - \left[ \frac{1}{\Gamma_{3r} \Gamma_{31} \Gamma_{32}} + \frac{1}{\Gamma_{r1} \Gamma_{3r} \Gamma_{2r}} + \frac{1}{\Gamma_{r1} \Gamma_{2r} \Gamma_{32}} \right. \\
 &\quad \left. + \frac{1}{\Gamma_{r1} \Gamma_{31} \Gamma_{2r}} + \frac{1}{\Gamma_{31} \Gamma_{32} \Gamma_{2r}} + \frac{1}{\Gamma_{32} \Gamma_{2r} \Gamma_{21}} \right].
 \end{aligned}$$

Equation (3.14) is close to the required form. It remains to show that  $Q_r(t)$  makes no contribution to  $\Delta p_r(t)$  in the long-time limit. The integrals over the level-broadened states can be performed in exactly the same way as we did for the  $N_{rr}(t)$  terms. Assuming Lorentzian profiles we obtain, in the long-time limit ( $\Gamma t \gg 1$ )

$$\begin{aligned}
 Q_r(t) &= -2g \sum_{q_1} \operatorname{Re} \left\{ \frac{V_{rq_1} \dot{p}_{rq_1}(0)}{E_{rq_1} + i\Gamma_{rq_1}} \right\} - 2g^2 \sum_{q_1} \sum_{q_2} \operatorname{Re} \left\{ \frac{V_{rq_2} V_{q_2 q_1} \dot{p}_{rq_1}(0)}{(E_{rq_1} + i\Gamma_{rq_1})(E_{rq_2} + i\Gamma_{rq_2})} \right. \\
 &\quad \left. - \frac{V_{rq_2} V_{q_1 r} \dot{p}_{q_1 q_2}(0)}{(E_{q_1 q_2} + i\Gamma_{q_1 q_2})(E_{r_1 q_2} + i\Gamma_{r_1 q_2})} \right\} + \dots \tag{3.19}
 \end{aligned}$$

The essential thing to notice about equation (3.19) is that it is independent of time. Thus by making  $t$  sufficiently large,  $N_r(t)$ , which is linear in  $t$ , can always be made to dominate  $Q_r(t)$ , which is time independent. Now if there exists a time interval  $\Delta t$



sufficiently large that  $Q_r(t + \Delta t) \ll N_r(t + \Delta t)$  but small enough that

$$[p_r(t + \Delta t) - p_r(t)]/p_r(t) \ll 1$$

then we can write

$$\frac{\Delta p_r(t + \Delta t)}{\Delta t} \equiv \frac{\delta p_r}{\delta t} = - \sum_{q_1} K(r, q_1)[p_r(t) - p_{q_1}(t)] \tag{3.20}$$

where  $\delta p_r/\delta t$  is a coarse-grained time derivative. This equation is our master equation for  $p_r(t)$ , with the kernel  $K(r, q_1)$  given by equation (3.15).

#### 4. Application to the coupled atom-radiation problem

In this section we shall apply the above master equation to a simple system. Our model is that of a single two-level atom interacting with a mode of the electromagnetic field in a cavity. The particular problem in which we are interested may be characterized by the so-called ‘adiabatic approximation’ for the time development of the density matrix in which the rate of atomic transitions is much greater than the rate of change of the field. In addition, the mean state of excitation of the atom is preserved over long times by an unspecified pumping mechanism, as would be provided, for instance, in a discharge tube.

We have already mentioned that in this case the level broadening may be attributed to the atomic levels being unstable with respect to transitions to lower levels unspecified, or to the electromagnetic field having a small spread in energies. In either case, the broadened states represent unobserved coordinates, or a ‘reservoir’. To be definite, we assume Lorentzian profiles for the broadening, and we need two half-widths,  $\Gamma_u$  and  $\Gamma_l$ , associated with the upper and lower atomic states respectively.

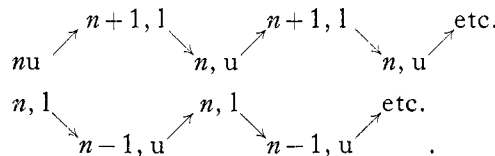
For simplicity, we assume resonance, i.e. that the unperturbed energies of the atomic and field quanta are the same. We shall not write out the reservoir interactions explicitly. The system Hamiltonian (using a system of units in which  $\hbar = 1$ ) is

$$H = (a^+ a + \frac{1}{2})\omega + \sigma_3\omega + (ga^+ \sigma_- + g^* a \sigma_+) \tag{4.1}$$

where  $a^+$  is the creation operator for a photon of energy  $\omega$ ,  $\sigma_+ = \sigma_x + i\sigma_y$ ,  $\sigma_- = \sigma_x - i\sigma_y$ ,  $\sigma_x$ ,  $\sigma_y$  and  $\sigma_3$  are the Pauli spin matrices. The final term in (4.1) represents the interaction between the field and the atom in the so-called rotating-wave approximation. This approximation results from using photon states with one component only of circular polarization.

We shall be concerned here only with deriving the equation satisfied by  $p_{r,r}(t)$ —the probability that there are  $n$  photons in the field at time  $t$ . For discussions of the nature of the solutions, see the papers listed under laser theory, or the review by Pike (1970).

Let  $|n, u\rangle$  be the state vector of the uncoupled system in which the atom is in its excited state and there are  $n$  photons in the field, and  $|n, l\rangle$  the vector when the atom is in its ground state with  $n$  photons in the field. In the system described by (4.1), the only transitions possible are of the type



The matrix elements of the interaction which we need are

$$\langle n, u | V | n+1, 1 \rangle = g^*(n+1)^{1/2} \quad (4.2)$$

$$\langle n, 1 | V | n-1, u \rangle = g\sqrt{n}. \quad (4.3)$$

We have already evaluated the quantity  $h(r, q)$  for a Lorentzian profile in equation (3.12), and it is straightforward to show that

$$h(r, q_1 q_2 q_3) = -\frac{1}{\Gamma_u \Gamma_1 (\Gamma_u + \Gamma_1)}.$$

Making use of the fact that, because of the special nature of the transition scheme, the third-order terms and fourth-order direct terms do not contribute, we can write down the master equations for  $p_{nu}(t)$  and  $p_{n+1,1}(t)$  from equation (3.20) as

$$\frac{\delta p_{nu}(t)}{\delta t} = -\frac{2|g|^2(n+1)}{\Gamma_u + \Gamma_1} \left\{ 1 - \frac{|g|^2(n+1)}{\Gamma_u \Gamma_1} \right\} [p_{nu}(t) - p_{n+1,1}(t)] \quad (4.4)$$

$$\frac{\delta p_{n,1}(t)}{\delta t} = -\frac{2|g|^2 n}{\Gamma_u + \Gamma_1} \left( 1 - \frac{|g|^2 n}{\Gamma_u \Gamma_1} \right) [p_{n,1}(t) - p_{n-1,u}(t)]. \quad (4.5)$$

It is important to remember that, because we are working with coarse-grained derivatives, the adiabatic approximation is already built into equations (4.4) and (4.5). (This means that we are observing the gross time behaviour of the system averaged over many lifetimes  $\Gamma_u^{-1}$  and  $\Gamma_1^{-1}$ . However, it is sometimes of interest to examine the time evolution of the system on a finer scale than this (see, for example, Haake 1969—in which the theory of the laser is developed beyond the adiabatic approximation).) We make the further approximations on the right-hand sides of (4.4) and (4.5), which are valid for weak coupling,

$$[p_{nu}(t) - p_{n+1,1}(t)] \simeq \sigma_u(t) \rho_n(t) - \sigma_1(t) \rho_{n+1}(t) \quad (4.6)$$

$$[p_{n,1}(t) - p_{n-1,u}(t)] \simeq \sigma_1(t) \rho_n(t) - \sigma_u(t) \rho_{n-1}(t) \quad (4.7)$$

where  $\sigma_u(t)$  and  $\sigma_1(t)$  are the average probabilities (over many lifetimes) of the atom being in its excited or ground state respectively at time  $t$ . We have assumed the existence of a pumping device which maintains the average atomic populations constant, therefore we can assume that  $\sigma_u(t) = \sigma_u$ ,  $\sigma_1(t) = \sigma_1$ .

The master function for the field is  $\rho_n(t) = \rho_{nu}(t) + \rho_{n,1}(t)$ . Substituting (4.6) and (4.7) into (4.4) and (4.5), and adding, we obtain an equation for  $\rho_n(t)$

$$\begin{aligned} \frac{\delta \rho_n(t)}{\delta t} = & -(n+1)(F_{n+1} \sigma_u) \rho_n(t) + (n+1)(F_{n+1} \sigma_1) \rho_{n+1}(t) \\ & - n(F_n \sigma_1) \rho_n(t) + n(F_n \sigma_u) \rho_{n-1}(t) \end{aligned} \quad (4.8)$$

where

$$F_n = \frac{2|g|^2}{\Gamma_u + \Gamma_1} \left( 1 - \frac{|g|^2 n}{\Gamma_u \Gamma_1} \right). \quad (4.9)$$

Equation (4.8) as it stands is sufficient to describe thermally generated light fields (Pike 1970) in a lossless cavity. In this case it is sufficiently accurate to take only the first-order term in  $|g|^2$  in  $F_n$ .

In a laser, where the atomic levels are maintained at an inverted population by pumping, it is necessary to retain the higher-order terms in (4.9). (Indeed, Scully and Lamb obtain  $F_n$  to all orders in  $|g|^2$  to describe the laser at high pumping levels.) We must also allow for the loss of radiation from the cavity (Pike 1970) by adding a term  $-Cn\rho_n$  to the right-hand side of equation (6). Since a loss of one photon from the  $(n+1)$ th level automatically means a gain in the occupation of the  $n$ th level we must also add a term  $C(n+1)\rho_{n+1}$ . Our final equation for the field density matrix of one atom interacting with a radiation field in a lossy cavity is then

$$\frac{\delta\rho_n(t)}{\delta t} = -(n+1)(F_{n+1}\sigma_u)\rho_n(t) + n(F_n\sigma_u)\rho_{n-1}(t) + (n+1)(F_{n+1}\sigma_1 + C)\rho_{n+1}(t) - n(F_n\sigma_1 + C)\rho_n(t). \quad (4.10)$$

We compare this equation with that of Scully and Lamb 1966)

$$\frac{d\rho_n(t)}{dt} = \frac{-A(n+1)}{1+(n+1)B/A}\rho_n(t) + \frac{An}{1+nB/A}\rho_{n-1}(t) - C_n\rho_n + C(n+1)\rho_{n+1}.$$

Bearing in mind that Scully and Lamb implicitly assume  $F_{n+1}\sigma_1 \ll C$ , our result agrees with the expansion of their equation to first order in  $B/A$  if we make the correspondences

$$A = \frac{2|g|^2\sigma_u}{\Gamma_u + \Gamma_1}, \quad B = \frac{2|g|^4\sigma_u}{\Gamma_u\Gamma_e(\Gamma_u + \Gamma_1)}.$$

Our derivation of this laser master equation using equation (3.20) above bypasses the *ab initio* calculation of Lamb and Scully and deals with the difficult question of irreversibility in the problem in a manner which is quite different in detail from that adopted by these authors. By emphasizing the concept of the master equation as the equivalent of the well-known and well-used perturbation series method, when working with quantum statistics and mixed states rather than quantum mechanics and pure states, we hope to have rendered its application more evident for this type of problem.

### Appendix

In this appendix we indicate how the simplification of  $N_{rr}(t)$  from the form given in (2.15) to that given in (2.17) is achieved. To do this we require the following mathematical identities:

$$U_1U_2 + U_2U_1 = (U_1)(U_2) \quad (A1)$$

$$U_1U_2U_3 = (U_1)(U_2U_3) - U_2(U_1)(U_2) \quad (A2)$$

$$U_1(U_2U_3) + U_2(U_1U_3) + U_3(U_2U_1) = (U_1)(U_2)(U_3) \quad (A3)$$

$$U_1U_2U_3U_4 = (U_1)(U_2U_3U_4) - U_2\{U_1(U_3U_4)\} \quad (A4)$$

$$U_1\{U_2(U_3U_4)\} = (U_1U_2)(U_3U_4) - U_3\{U_4(U_1U_2)\}. \quad (A5)$$

These relations are easily proved by integration by parts. As an example, we prove

the first:

$$\begin{aligned}
 U_1 U_2 &= \int_0^t dt_1 V_1(t_1) \int_0^{t_2} dt_2 V_2(t_2) \\
 &= \left[ \int_0^{t_1} dt' V_1(t') \int_0^{t_1} dt_2 V_2(t_2) \right]_{t_1=0}^{t_1=t} - \int_{t_1=0}^{t_1=t} dt_1 \left( \int_0^{t_1} V_1(t') dt' \right) V_2(t_1) \\
 &= \int_0^t dt_1 V_1(t_1) \int_0^t dt_2 V_2(t_2) - \int_0^t dt_1 V_2(t) \int_0^{t_1} V_1(t_2) dt_2
 \end{aligned}$$

i.e.

$$= (U_1)(U_2) - U_2 U_1.$$

To obtain the first term in (2.17) it is necessary to show that

$$U_{rq_1} U_{q_1 r} + U_{rq_1} U_{q_1 r} = (U_{rq_1})(U_{q_1 r}).$$

This is just the relation (A1) with  $rq_1 = 1$ ,  $q_1 r = 2$ . Similarly, to establish the second term of (2.17) we first rewrite the third term of  $N_{rr}(t)$  given by (2.15) as

$$\begin{aligned}
 &\sum_{q_1} \sum_{q_2} \{ U_{rq_2} U_{q_2 q_1} U_{q_1 r} - U_{q_2 r} U_{q_1 q_2} U_{rq_1} \} p_r(0) \\
 &\quad + (-U_{rq_2} U_{q_2 q_1} U_{q_1 r} - U_{rq_2} U_{q_1 r} U_{q_2 q_1} + U_{rq_1} U_{q_2 r} U_{q_1 q_2} + \text{h.c.}) p_{q_1}(0).
 \end{aligned}$$

By using (A2) and (A1) the first contribution can be written as

$$\sum_{q_1} \sum_{q_2} \{ -(U_{rq_2})(U_{q_1 r} U_{q_2 q_1}) + (U_{q_1 r})(U_{rq_2} U_{q_2 q_1}) \} p_r(0).$$

We can interchange  $q_1$  and  $q_2$  in the first term, when the expression reduces to

$$\sum_{q_1} \sum_{q_2} \{ (U_{q_1 r})(U_{rq_2} U_{q_2 q_1}) - (U_{rq_1})(U_{q_2 r} U_{q_1 q_2}) \} p_r(0). \quad (\text{A6})$$

The second contribution is likewise reduced by using first (A1), then (A2). The result is

$$\sum_{q_1} \sum_{q_2} \{ (U_{q_1 r})(U_{rq_2} U_{q_2 q_1}) + (U_{rq_1})(U_{q_2 r} U_{q_1 q_2}) \} p_{q_2}(0). \quad (\text{A7})$$

(A6) and (A7) together give the second term of (2.17). The third term of (2.17) can also be obtained by using the relations (A1)–(A5).

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